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Effects of the coating system and interfacial region thickness on the thermal residual stresses in SiC_f/Ti–6Al–4V composites

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A three-dimensional finite element model was developed to study effects of the coating system and interfacial region thickness on the distributions of the thermal residual stresses in continuous SiC fiber reinforced Ti–6Al–4V composite. Three coating systems were applied in this study, that is, C coating, C/TiB_2 coating and without coating. The influence of the interfacial region thickness on the thermal residual stresses in the composite was analyzed with concerning the simple case of without coating. Some proposal was given for the interface structure design of the composites. With regard to the thermal residual stresses, the C coating is an advisable choice for the interface structure design of the continuous SiC fiber reinforced Ti–6Al–4V composites. And for the region of the interfacial region thickness from 1 μm to 3 μm, the thicker interfacial region can reduce most of the thermal residual stresses in composites and improve the axial tensile strength of the composite.

1. Introduction

Continuous SiC fiber reinforced Ti alloy matrix composites (Ti-MMCs) are potential materials for using in the aerospace industry and other high-technology fields owing to their low density, high performance and high specific strength at room and elevated temperature [1–3]. However, the thermal residual stresses caused by the mismatch in the coefficient of thermal expansion (CTE) between the Ti alloy matrix and the SiC fiber reinforcement during the cooling from the consolidation temperature influence the overall mechanical properties of the composites [4]. Therefore, there has been considerable interest in the thermal residual stresses of the Ti-MMCs. At the same time, in the composites, an interfacial region (i.e. an interface coating or an interfacial reaction layer) between the fiber and matrix with a finite thickness is known to exist. The thermal residual stresses in the interfacial region have a significant influence on the composite properties [5–10]. Consequently, more attentions have been focused on the thermal residual stresses near the interfacial region in SiC_f/Ti–6Al–4V composites. Shaw and Miracle [5] have studied the effect of the interfacial region on the transverse behavior of metal–matrix composites using the finite element analysis (FEA). In their model, Yttria coated, graded carbon coated and without coated interface have been considered independently. Their results shown the thermal residual stresses in the interfacial region strongly depend on the properties of the interfacial region, while the residual stresses in the matrix and fiber are not significantly affected by these properties. And they believed the thickness of the coating has little influence on the thermal residual stresses. Robertson and Mall [6] have examined the effect of the thickness of the interfacial region on transverse properties of titanium-based metal–matrix composites. However, the matrix is assumed to be elastic in the model. Haque and Choy [7] have investigated the effect of the coating on thermal residual stresses generated at the fiber/matrix interface due to differences in the CTE mismatch between the various materials within the coating system. Numerical modeling of composites with a finite thickness interface has also been carried out by Broutman and Agarwal [8]. However, their analyses are limited by the assumption of linear elastic behaviors of all constituents (i.e. fiber, matrix and interfacial region) and only longitudinal properties are evaluated. Xia et al. [9] investigated the axial stresses in composites by using a three-dimension (3D) finite element model with concerning the interfacial reaction layer thickness. Meinhard et al. [10] obtained the interfacial region has an outstanding effect on the thermal residual stresses in composites by introducing a four-phase model consisting of concentric cylinders which represent fiber, interfacial layer, matrix and composite.

In this paper, the attention is focused on simulating the thermal residual stresses in the SiC_f/Ti–6Al–4V composite system by using a 3D model with concerning the different coating systems and thicknesses of interfacial region. Based on this analysis, a guideline for the coating system and interfacial region thickness selections is proposed to improve performances of the composites.

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2. Finite element analysis

2.1. Properties of the composite constituents

The composite system consists of a titanium alloy matrix, Ti–6Al–4V, reinforced by SiC fibers with a volume fraction of 20% and an interfacial region. In this system, the SiC fibers were treated as elastic and transversely isotropic (Table 1), whereas time independent elastic–plastic behavior was used to describe the isotropic Ti–6Al–4V matrix (Table 2). In Table 1, the subscript T and A denote the transverse and axial direction, respectively.

In earlier works, the coated fiber reinforced titanium alloy matrix composites have been studied by using theoretical modeling [7] and experimental [11–14]. The C coating and C/TiB_2 double coating were mostly investigated in these papers. The C coating prevents the direct reaction between the fiber and matrix and produces the brittle TiC between C coating and matrix. Therefore, the interfacial region can be simulated as C/TiC in case of C coating. Mogilevsky [14] obtained the TiB_2/matrix interface may be unstable both thermo-dynamically and kinetically and the kinetic instability manifest itself in the growth of TiB needles at the TiB_2/matrix interface. However, in this analysis, the interfacial region can be simulated as C/TiB_2 in case of C/TiB_2 coating without concerning the TiB needles because TiB needles cannot form a separated layer. In addition, for the fibers without coating, according to Lü [15], the magnitude of TiC is the greatest among the interfacial reaction products. Consequently, the composition of the interfacial region was nearly treated as TiC in case of without coating in the analysis. As described above, the interfacial region can be simulated as C/TiC, C/TiB_2 and TiC in case of C coating, C/TiB_2 coating and without coating, respectively in this analysis. And C, TiC and TiB_2 were treated as elastic and isotropic. Their thermal and mechanical properties are shown in Table 3.

2.2. 3D finite element model

Finite element analysis was implemented using the ANSYS code. A 3D model with a square fiber array included three phases, i.e. the fiber, interfacial region and matrix, and two distinct interfaces, one between the fiber and interfacial region (f/i interface) and the other between interfacial region and matrix (i/m interface). As shown in Fig. 1, the representative volume element (RVE) was selected to predict the thermal residual stresses in SiC_f/Ti–6Al–4V composite. The global behavior of the composite was assumed to be same as that of RVE. The fiber was 140 μm in diameter. Along the fiber direction, the model thickness was

Table 1
SiC fiber properties used in the model

Material	Young's modulus (GPa)		Shear modulus (GPa)		Poisson ratio		Coefficient of thermal expansion (10^{-6}/°C)	
SiC	E_T	E_A	G_T	G_A	ν_T	ν_A	α_T	α_A
	262.6	403.2	109.5	93.1	0.194	0.148	2.63	4.5

Table 2
Ti–6Al–4V properties used in the model

Temperature (°C)	Young's modulus (GPa)	Poisson ratio	Yield stress (MPa)	Flow modulus (GPa)	Coefficient of thermal expansion (10^{-6}/°C)
23	125	0.31	1000	0.7	8.7800
260	110	0.31	630	2.2	9.8300
427	100	0.31	525	2.2	10.710
538	74	0.31	446	1.9	11.220
650	55	0.31	300	1.9	11.680
800	27	0.31	45	2	12.210

Table 3
C, TiB_2 and TiC properties used in the model

Material	Temperature (°C)	Young's modulus (GPa)	Poisson ratio	Coefficient of thermal expansion (10^{-6}/°C)
C	All temperature	160	0.23	10.0000
TiB_2	All temperature	569	0.113	8.1000
TiC	All temperature	440	0.2	7.6000

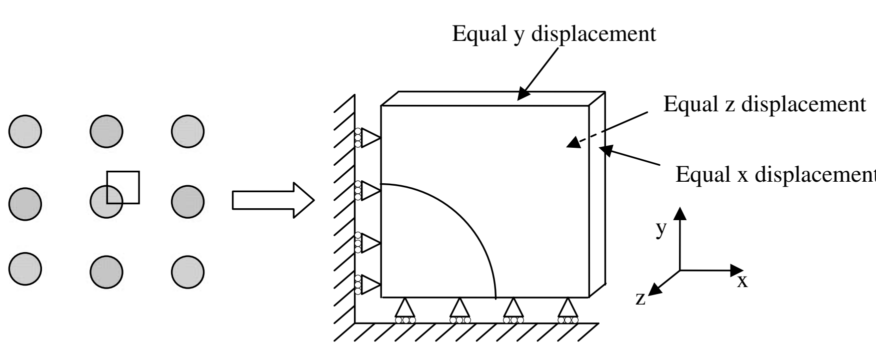

Fig. 1. Fiber arrangement, selected RVE and boundary conditions.

1 μm. The nodes on the bottom face of the model (i.e. the *x*–*z* plane at $y = 0$) were not allowed to move in the *y*-direction, while the nodes on the top face of the model were coupled together to shift an equal amount of displacement in the *y*-direction. Similarly, the nodes on the front face of the model (i.e. the *y*–*z* plane at $x = 0$) and on the left face of the model (i.e. the *x*–*y* plane at $z = 0$) were not allowed to move in the *x*-direction and *z*-direction, respectively, while the nodes on the back and right face of the model were coupled together to shift an equal amount of displacement in the *x*-direction and *z*-direction, respectively. Furthermore, the node at the origin of the model was not allowed to move in any direction to prevent rigid body displacement. The f/i interface and i/m interface were assumed to be perfectly bonded. Fig. 2 shows the complete geometry of the model and the finite element mesh.

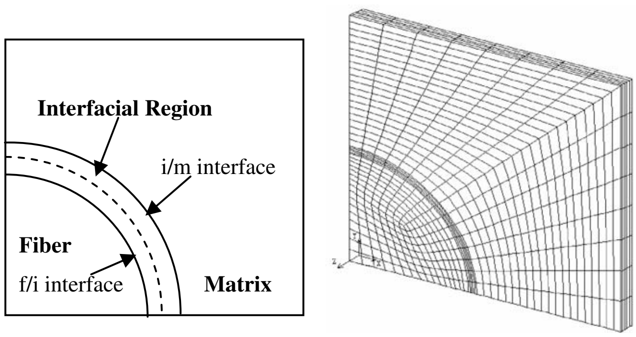

Fig. 2. Geometry details of the composite constituents and finite element mesh of the RVE.

Because an analysis starting from the processing temperature would predict unrealistically large residual stresses and strain, the prediction was started from a stress-free temperature of 700 °C and cooled to 25 °C [16]. Three dimensional eight nodes elements SOLID45 were used to construct in the analysis.

As the influence of the coating system on the thermal residual stresses in composites was analyzed, the interfacial region thickness in the model was assumed as constant 3 μm. As mentioned before, in case of C coating, the interfacial region can be simulated as C/TiC. Simplicity, the thickness ratio of C and TiC was equal to 1 (i.e. the thickness of C was 1.5 μm and equal to the thickness of TiC). Similarly, In case of C/TiB_2 coating, the thickness ratio of C and TiB_2 was equal to 1. Obviously, in case of without coating, the interfacial region was only 3 μm thick TiC. As the influence of the interfacial region thickness on the thermal residual stresses was discussed, the case of without coating was applied. And the region of the interfacial region thickness is from 1 μm to 3 μm.

3. Results and discussion

3.1. The influence of the coating system

As shown in Fig. 3, the thermal residual stresses in composites were plotted as a function of the radial distance. As can be observed, in the interfacial region, the coating system has a significant influence on the hoop stresses. Both in case of C coating and C/TiB_2 coating, the hoop stresses in the interfacial region have a peak in the layer adjacent to the matrix. Differently, the stress peak in TiB_2 layer is higher than that in TiC layer. On the contrary, in case of without coating, the hoop stresses in the interfacial region

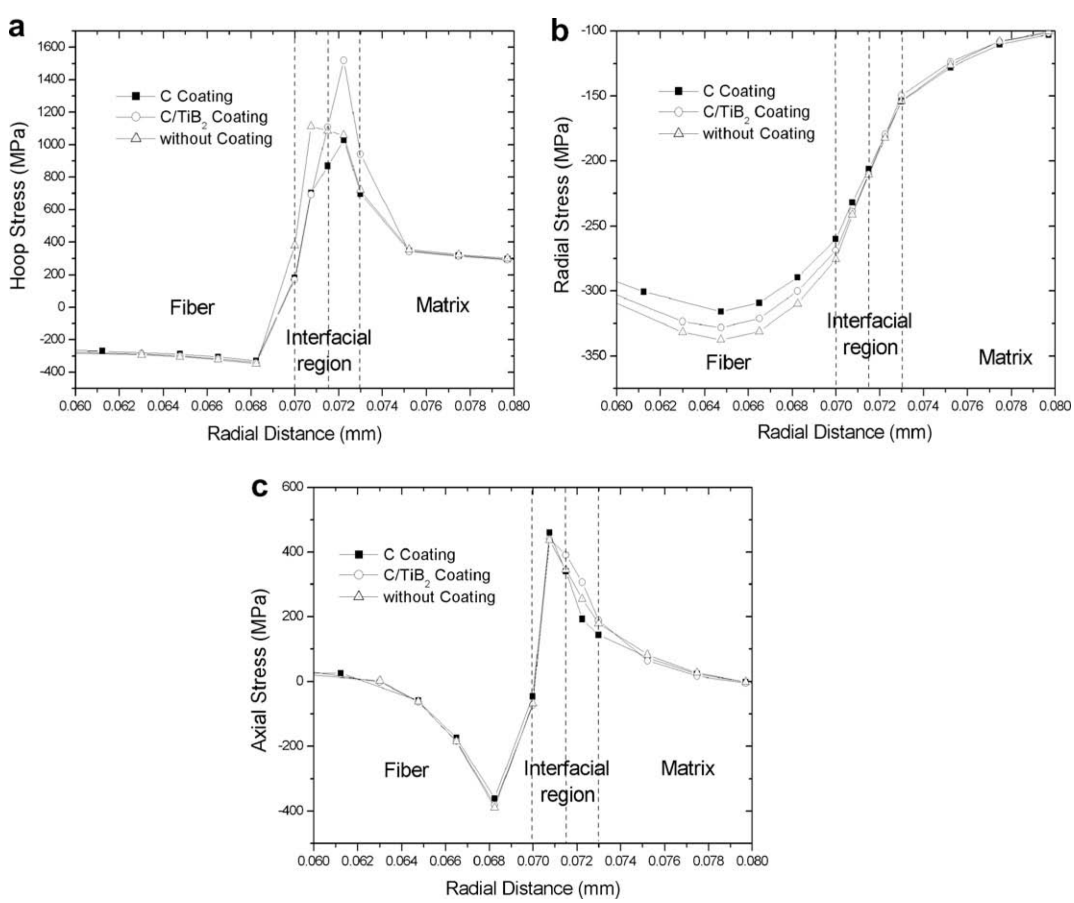

Fig. 3. Distributions of the thermal residual stresses along radial direction with the different coating system: (a) hoop stress, (b) radial stress and (c) axial stress.

are nearly constant and between that in case of C coating and C/TiB_2 coating. In addition, the value of the hoop stresses is very high in the interfacial region and matrix adjacent to the interfacial region, even close to 1200 GPa. The high hoop stresses generally make the cracks take place easily perpendicular hoop direction in this zone during the composite fabrication process. The radial stresses in the interfacial region are nearly independent of the coating system. The coating system has a little influence on the axial stresses in the interfacial region as seen in Fig. 3c. In the interfacial layer adjacent to the fiber, the axial stresses are independent of the coating system. However, in the interfacial layer adjacent to the matrix, the axial stresses in case of C/TiB_2 coating are higher than in case of other coating system. And the axial stresses are lowest in case of C coating. From Fig. 3, the coating system has little influence on the thermal residual stresses in the fiber and matrix except for the radial stresses in the fiber. The radial compressive stresses in the fiber are highest in case of without coating, lowest in case of C coating and medium in case of C/TiB_2 coating.

Generally, the larger CTE mismatch between components, the higher stresses in composites. As described in Tables 1–3, the

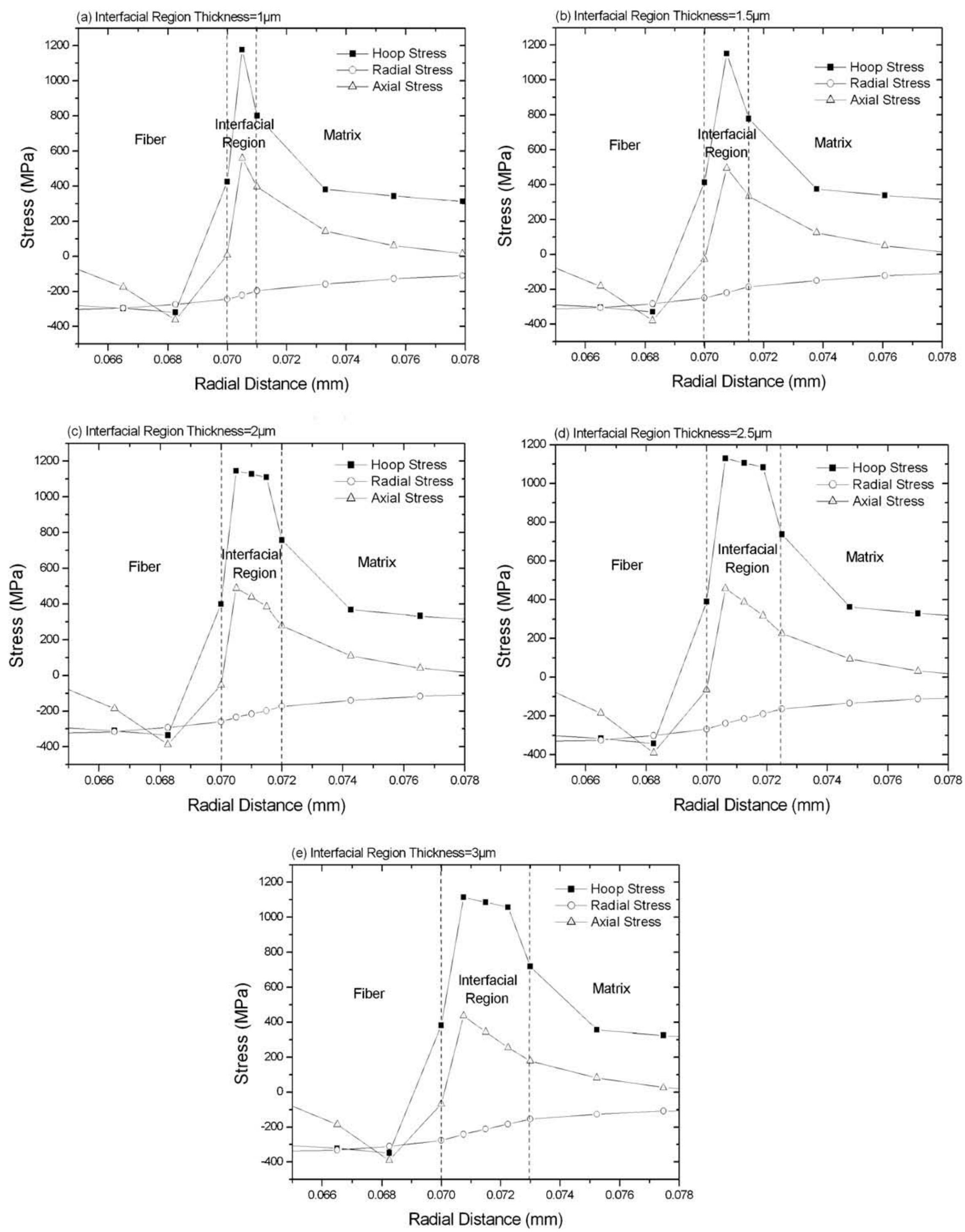

Fig. 4. Distributions of the thermal residual stresses as a function of radial direction with the different interfacial region thickness: (a) 1 μm, (b) 1.5 μm, (c) 2 μm. (d) 2.5 μm and (e) 3 μm.

transverse CTE mismatch between the fiber and C is larger than that between the fiber and TiC, whereas the transverse Young's modulus mismatch between the fiber and C is lower than that between the fiber and TiC. In fact, in Fig. 3a, the hoop stresses in the interfacial layer adjacent to the fiber and at the f/i interface in case of C and C/TiB_2 coating are lower than in case of without coating. Similar phenomenon exists in the interfacial layer adjacent to the matrix and at the i/m interface. Therefore, the hoop stresses in the interfacial region are mostly dependent upon rather the Young's modulus than CTE mismatch between the components. In Fig. 3b, the radial stresses in the interfacial layer adjacent to the fiber and at the f/i interface in case of C and C/TiB_2 coating are lower than in case of without coating because of the soft C coating. Simultaneously, the radial stresses in the interfacial layer adjacent to the fiber and at the f/i interface in case of C coating are lower than in case of C/TiB_2 coating. The result can be mostly contributed to the higher Young's modulus of TiB_2 than TiC in the interfacial region. The similar phenomenon also exists in the fiber. As well as the hoop stresses, the influence of the CTE mismatch on the radial stresses is inconspicuous. However, in general, the influence of the coating system on the radial stresses is negligible. In Fig. 3c, the influence of the coating system on the axial stresses is visible only in the interfacial layer adjacent to the matrix. The axial stresses in case of C/TiB_2 coating are highest because of the high Young's modulus of TiB_2. Although the compositions of the interfacial layer adjacent to the matrix are TiC both in case of C coating and without coating, the soft C layer reduce the CTE and Young's Modulus mismatch between the fiber and TiC. Therefore, the axial stresses in the interfacial layer adjacent to the matrix in case of C coating are lower than in case of without coating. Also it can be seen from Fig. 3c, the axial stresses in the fiber, matrix and the interfacial layer adjacent to the fiber are independent of the coating system.

3.2. The influence of the interfacial region thickness

The distributions of the thermal residual stresses as a function of radial distance with different interfacial region thicknesses are illustrated in Fig. 4. It can be seen from Fig. 4, the radial stresses in the composite are independent of the interfacial region thickness as the thickness increases from 1 μm to 3 μm. However, the interfacial region thickness has an outstanding influence on the hoop and axial stresses in the composite. In the interfacial region, the hoop and axial stresses decrease with increasing the interfacial region thickness. This result can be mostly contributed to the reduction of the stress concentration at the interfacial region as the interfacial region thickness increases. In addition, it is notable that the axial stresses in the interfacial region have a sharper decrease along radial direction than the hoop stresses. At the i/m interface, the hoop and axial stresses also decrease with increasing the interfacial region thickness. Remarkably, the axial stresses have a more notable reduction than the hoop stress at the i/m interface with increasing the interfacial region thickness. At the f/i interface, the hoop stresses are nearly constant with increasing the interfacial region thickness. However, the axial compressive stresses increase with increasing the interfacial region thickness. The high axial compressive stresses at the f/i interface can improve the axial tensile strength of the composite. In the fiber and matrix, the thermal residual stresses are nearly independent of the interfacial region thickness. In addition, the radial stresses have an agreement with the hoop stresses in the fiber.

4. Conclusions

The coating system has a significant influence on the thermal residual stresses (especially on the hoop stresses) in the interfacial region instead of the fiber and matrix in the composites. Simultaneously, the hoop stresses in the interfacial region are mostly dependent upon rather the Young's modulus than CTE mismatch between the components within the coating system. With regard to the thermal residual stresses in composites, the C coating is an advisable choice for the interface structure design of the composites. Whether the C/TiB_2 coated fibers or without coated fibers make a high stress level in the interfacial region.

The radial stresses in the composite are independent of the interfacial region thickness as the thickness increases from 1 μm to 3 μm. However, in the interfacial region, the hoop and axial stresses decrease with increasing the interfacial region thickness. In the fiber and matrix, the thermal residual stresses are nearly independent of the interfacial region thickness as the thickness increases from 1 μm to 3 μm. For the region of the interfacial region thickness from 1 μm to 3 μm, the thicker interfacial region can reduce most of the thermal residual stresses in composites and improve the axial tensile strength of the composite.

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